## Professor Rosa M<sup>a</sup> Claramunt

## A tribute



This special issue of Arkivoc is dedicated to Professor Rosa M<sup>a</sup> Claramunt to commemorate her 65<sup>th</sup> birthday and to acknowledge her contribution to heterocyclic organic chemistry.

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Rosa M<sup>a</sup> Claramunt was born in Molins de Rei on April 29, 1948. She studied Chemistry at the University of Barcelona where she graduated in 1969.

Before completing her degree, Rosa began her scientific career in the Faculty of Chemistry. After graduation she was appointed Assistant Professor and elaborated her PhD Thesis *"Synthesis and Physicochemical Studies of Nitrogenous Heterocyclic Compounds"* as part of a scientific research project carried out between the Universities of Barcelona and Montpellier. As a result of that collaboration she was awarded her PhD from the University of Barcelona in 1973 and defended a Diplôme d'Études Approfondies and a Thèse d'État at the University of Montpellier in 1971 and 1976, respectively.

From 1974 she spent five years as a postdoctoral fellow in several universities; at the University of East Anglia University (UK), in the research group of Professors Alan R. Katritzky and John Boulton; at the Université de l'État à Mons (Belgium), in the group of Professors André Maquestiau and Robert Flammang; at the University of Lund (Sweden), in the group of Professor Jan Sandström and at the University of Aix-Marseille (France) and during the last four years in the group of Professor Jacques Metzger.

In 1979 she returned to Spain and was appointed Associate Professor of Organic Chemistry at the Universidad Nacional de Educación a Distancia (UNED). At this time, UNED did not have a research laboratory so in 1980 she was appointed Associate Doctor at the Institute of Medicinal

Chemistry, which belongs to the CSIC, where she developed her first investigation project, entitled "*Synthesis of Biologically Active Adamantyl Heterocycles*", funded by the Spanish Ministry of Education. This project set the basis for her future involvement in the design of heterocycles with biological properties. In 1986, she was promoted to Full Professor in Organic Chemistry at the UNED. She became very active in fund raising to create a technical and scientific infrastructure in order to improve the research activity in the chemistry department at UNED, which led to more than 400 papers.

Her *curriculum vitae* reflects her capacity, tenacity and boldness to achieve and maintain a top tier scientific research activity through 30 years of dedication to Science in Spain, including cooperation with foreign universities. She directed a large amount of research by PhD students and professors, from France, Argentina, Germany, Morocco, Slovakia, Cuba, among others.

Rosa Claramunt's first paper reported the synthesis of norpethidine derivatives (1971); it was prepared in collaboration with the only Spanish laboratory allowed to work on controlled drugs. Her second paper, also written in 1971 dealt with research carried out under the direction of the late Professor Robert Jacquier (University of Montpellier); it described the use of shift reagents that initiated Rosa Claramunt's continued interest in NMR. Discussing a *curriculum* that covers about 400 papers is difficult, but here is a classification of her main interests:

**1. Heterocyclic Chemistry.** From her first paper (1971OMR595) to her last one [2012ARK(ii)85], many heterocyclic compounds have been prepared, structurally characterized and their biological properties determined. Pyrazoles, indazoles, imidazoles, benzimidazoles, 1,2,4-triazoles, 1,2,3-triazoles, benzotriazoles, tetrazoles, *N*-acylazoles (azolides, review year 2000), azapentalenes (including a review in *Adv. Heterocycl. Chem.* 1978), polyazolylmethanes (including their coordination chemistry), polyazolylbenzenes (aromatic propellenes, with a 1997 review), pyridinium salts, perimidines, scorpionates, ... Many were devoted to tautomerism (including a review in *Adv. Heterocycl. Chem.* 2000),. The systematic exploration of the effect of fluorine substituents on the physicochemical and biological properties of heterocycles deserves special mention.

**2.** Adamantane. Amongt the substituents of these heterocycles, Rosa Claramunt explored the 1adamantyl substituent with special care. No less than 18 papers were devoted to different aspects of this singular substituent: 1-(1-adamantyl)azoles and benzazoles, antiviral activity, crystallography, NMR spectroscopy,  $\pi$  values, flash vacuum pyrolysis. During the preparation of *N*-adamantyl-pyrazoles, one of the most remarkable microwave heating effects was discovered.

**3. NMR spectroscopy in the UNED group** directed by Rosa Claramunt is used not only as an analytical tool to characterize compounds but as a physicochemical method to explore the properties of molecules. To this end, all the nuclei accessible to their instruments have been used leading to some significant discoveries.

**4. Host-guest Chemistry.** A research line of increasing importance is the study of the interactions between small and large molecules, an important part of supramolecular chemistry. Both in the solid state (CPMAS-NMR, DSC and crystallography) and in solution (NMR), the

complexes formed by ureas with a variety of synthetic hosts have been studied. In this work, the primordial role played by hydrogen bonds was carefully analyzed.

**5. Medicinal Chemistry.** Along the years and related to external inputs (collaboration with South American Universities, industry contracts, ...) a series of drugs have been studied. For instance, Nifurtimox, Nitrofurfural, Allopurinol, antichagasic drugs, carbon anhydrase activators, Tolbutamide, Alloxazine, Curcuminoids, NOS inhibitors (this being one of the most systematically explored), Omeprazol, Glicazide, Glibenclamide and antibacterial quinolones.

It is important to mention that she was the female representative of the "Real Patronato de la Biblioteca Nacional de España" from 2006 to 2009, in acknowledgement of her professional career. It is also important to highlight that Professor Claramunt is responsible scientific investigator, who is the role model and engine of the consolidated Scientific Research group of the UNED "*Supramolecular Bioorganic Systems*".

On a personal level she lives in a scientific atmosphere. Her husband, José Elguero, is an acknowledged scientist in Physical Organic Chemistry. They have a son, David, also a chemist, and a daughter, Isabel, veterinarian, who prefers working in open spaces rather than a laboratory. During vacation periods, Rosa enjoys spending time with her family in her place of birth, Catalonia, near the Mediterranean Sea. She reads a lot and is a theatre fanatic, but what she loves most is films. Amongst her numerous skills, we should emphasize her creativity, optimism, tenacity and overall her exceptional human quality which is reflected by her family, friends and colleagues who love her.

It is a pleasure for me to participate in this commemorative issue. I met Rosa more than 30 years ago. She has been my research mentor, colleague and friend during all these years. I hope she continues to promote the development of Heterocyclic Chemistry and remains a role model for all scientist women who admire her contribution to science.

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## Some Recent Publications of Prof. Rosa M<sup>a</sup> Claramunt

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- 3. Uldry, A-CH.; Griffin, J. M.; Yates, J. R.; Pérez-Torralba, M.; Santa María, M. D.; Webber, A. L.; Beaumont, M. L. L.; Samoson, A.; Claramunt, R. M.; Pickard, CH. J.; Brown, S. P.

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- 7. Cornago, P.; Claramunt, R. M.; Bouissane, L.; Alkorta, I.; Elguero, J. A study of the tautomerism of  $\beta$ -dicarbonyl compounds with special emphasis on curcuminoids. *Tetrahedron* **2008**, *64*, 8089.
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- 10. Pérez Medina, C.; López, C.; Claramunt, R. M.; Elguero, J. Trifluoro-3-hydroxy-1*H*indazolecarboxylic acids and esters from perfluorinated benzenedicarboxylic acids. *Eur. J. Org. Chem.* **2010**, 890.
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15. Alkorta, I.; Sánchez-Sanz, G.; Trujillo, C.; Elguero, J.; Claramunt, R. M. A theoretical study of the parent N*H*-benzazoles (benzimidazoles, indazoles and benzotriazoles): Geometries, energies, acidity and basicity, NMR properties and molecular electrostatic potentials. Dedicated to Prof. Anthony J. Arduengo on the occasion of his 60<sup>th</sup> anniversary. *ARKIVOC* **2012**, *ii*, 85.